4-«alpha»,7-Epoxy-11-methoxy-10-«beta»-H-spiro

Inchi: InChI=1S/C16H26O2/c1-12-7-6-8-14(4)15(12)9-10-16(11-15,18-14)13(2,3)17-5/h6,8,12H
InchiKey: DPCMNLDHVSKLRP-YUCHNRCRSA-N
Formula: C16H26O2
SMILES: COC(C)(C)C12CCC3(C1)C(C)CC=CC3(C)O2
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	59.39	kJ/mol	Joback Method
hf	-357.30	kJ/mol	Joback Method
hfus	12.55	kJ/mol	Joback Method
hvap	53.45	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.705		Crippen Method
mcvol	211.160	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1595.00		NIST Webbook
tb	635.59	K	Joback Method
tc	872.70	K	Joback Method
tf	436.30	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.01	J/mol×K	635.59	Joback Method
cpg	642.14	J/mol×K	675.11	Joback Method
cpg	663.12	J/mol×K	714.63	Joback Method
cpg	683.43	J/mol×K	754.15	Joback Method
cpg	703.56	J/mol×K	793.67	Joback Method
cpg	723.98	J/mol×K	833.18	Joback Method
cpg	745.18	J/mol×K	872.70	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R236052&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume